

OFFICE OF NAVAL RESEARCH

CONTRACT N00014-95-1-0028

R&T Code 4131D02

Dr. Richard S. Miller

Technical Report No. 76

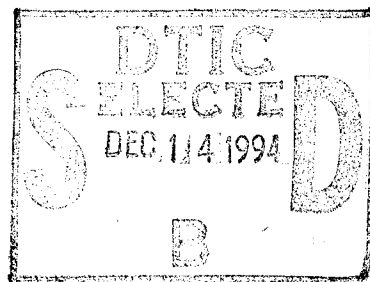
CONTINUED COMPUTATIONAL EVALUATION OF THE
FEASIBILITY OF NITRATING PRECURSORS TO $C_{12}N_{12}O_{12}$.

by

Peter Politzer and M. Edward Grice

Department of Chemistry
University of New Orleans
New Orleans, LA 70148

December 5, 1994

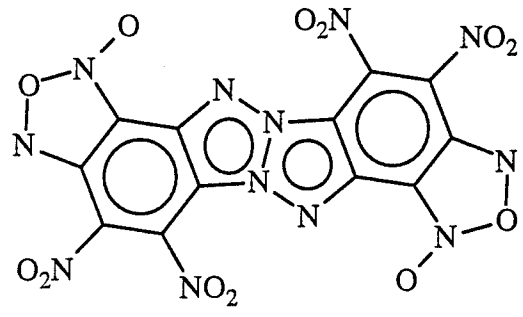


Reproduction in whole or in part is permitted for any purpose of the United States Government.

This document has been approved for public release and sale; its distribution is unlimited.

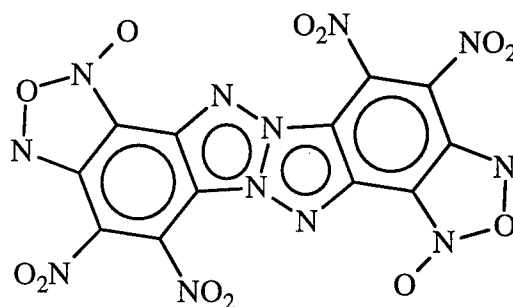
19941209 064

DTIC QUALITY INSPECTED 1

REPORT DOCUMENTATION PAGE			Form Approved OMB No. 0704-0188	
Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503.				
1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE December 5, 1994	3. REPORT TYPE AND DATES COVERED Technical Report		
4. TITLE AND SUBTITLE Continued Computational Evaluation of the Feasibility of Nitrating Precursors to $C_{12}N_{12}O_{12}$		5. FUNDING NUMBERS N00014-95-1-0028 Dr. Richard S. Miller R& T Code 4131D02		
6. AUTHOR(S) Peter Politzer and M. Edward Grice		8. PERFORMING ORGANIZATION REPORT NUMBER		
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) University of New Orleans Department of Chemistry New Orleans, Louisiana 70148		10. SPONSORING/MONITORING AGENCY REPORT NUMBER		
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) Offie of Naval Research Code 333 800 N. Quincy Street Arlington, VA 22217		11. SUPPLEMENTARY NOTES		
12a. DISTRIBUTION / AVAILABILITY STATEMENT Approved for public release. Unlimited distribution.		12b. DISTRIBUTION CODE		
13. ABSTRACT (Maximum 200 words) <p>Extending the work reported in Technical Report No. 71 (October 20, 1994), we computed the average local ionization energies on the surfaces of two more possible precursors to 1. No minima were found at the positions to be nitrated, indicating that these are not favored sites for this purpose.</p> <div style="text-align: center; margin: 10px 0;">  </div>				
14. SUBJECT TERMS $C_{12}N_{12}O_{12}$, nitration, average local ionization energies			15. NUMBER OF PAGES 3	
17. SECURITY CLASSIFICATION OF REPORT Unclassified			16. PRICE CODE	
18. SECURITY CLASSIFICATION OF THIS PAGE Unclassified		19. SECURITY CLASSIFICATION OF ABSTRACT Unclassified		20. LIMITATION OF ABSTRACT Unlimited

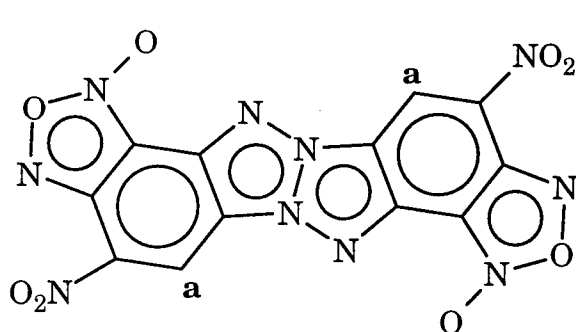
Introduction

In Technical Report No. 71 (October 20, 1994), we investigated the susceptibility to electrophilic attack involving charge transfer (as in nitration) of several possible precursors to **1**. We computed the average local ionization energies $\bar{I}_S(r)$ on the surfaces of **2** - **4** (Figure 1) in order to determine the ease of charge transfer at positions **a** and **b**. At the request of M. L. Trudell, we have now extended this study to include **5** and **6**. The procedure used was the same as described in the earlier report, which also discusses the definition and interpretation of $\bar{I}_S(r)$. The results are given in Figure 1, together with those obtained previously.

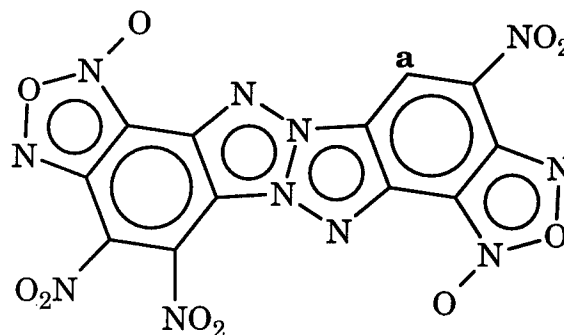


1

We find no minimum in $\bar{I}_S(r)$ at positions **a** in **5** and **6**, which is consistent with what was observed earlier for **4**. This indicates that these are not favorable sites for charge transfer to an electrophile.



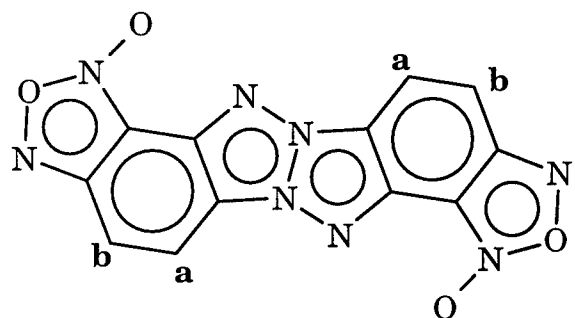
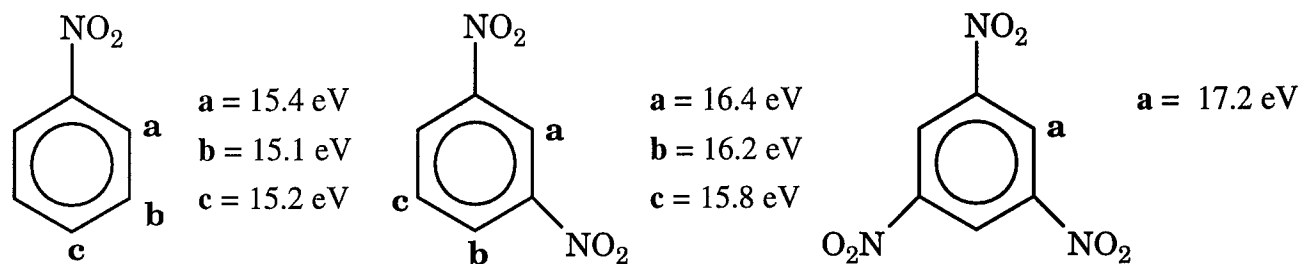
5



6

Accession For	
WHS GRAB	<input checked="" type="checkbox"/>
WHS LAB	<input type="checkbox"/>
Unassigned	<input type="checkbox"/>
Justification	
By _____	
Distribution _____	
Availability Order	
Dist	Special
A-1	

Figure 1. Some Computed (STO-5G) Minima of Average Local Ionization Energies on Molecular Surfaces

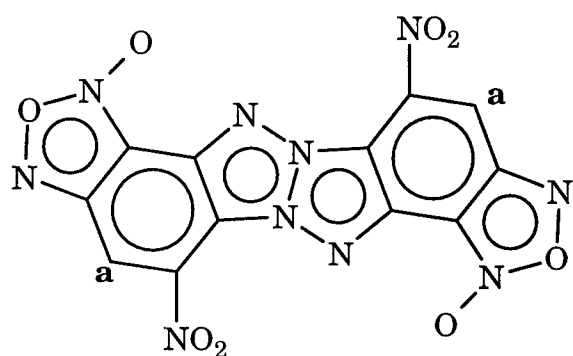


4

a: no minimum;

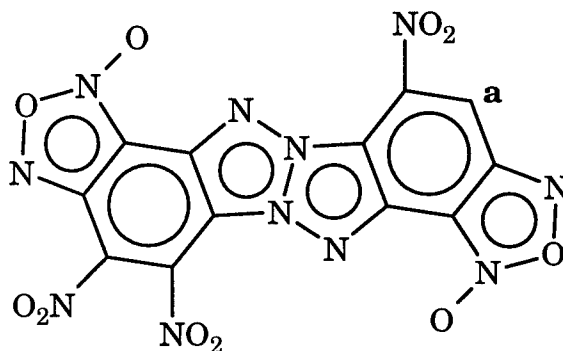
 $\bar{I}_S(r) = \text{approx. } 15.9 \text{ eV.}$

b = 15.2 eV



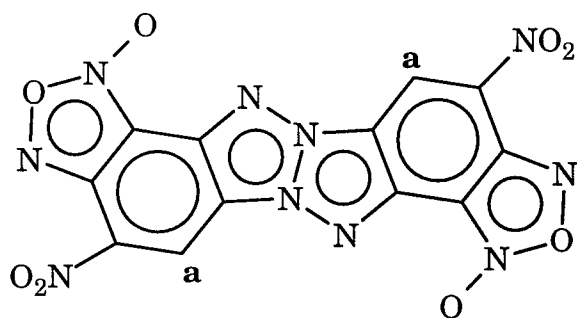
2

a = 16.3 eV



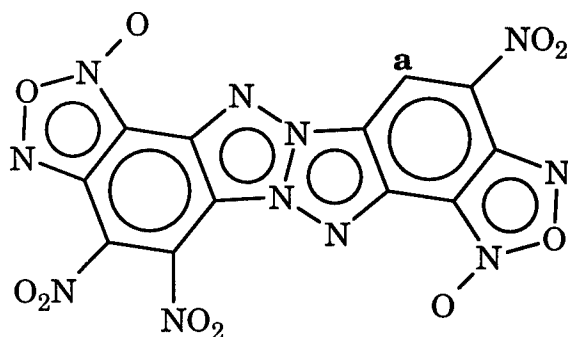
3

a = 16.6 eV



5

a: no minimum;

 $\bar{I}_S(r) = \text{approx. } 16.8 \text{ eV.}$ 

6

a: no minimum;

 $\bar{I}_S(r) = \text{approx. } 17.0 \text{ eV.}$